



## Glenn T. Seaborg Center Seminar

### **First-Principles Calculations for Lanthanides and Actinides: Applications to Eu-based New Gamma Ray Detectors and Energy Critical Materials**

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***Computational Research Division  
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**Wednesday, September 5, 2012  
4:00 - 5:00 pm  
Bldg. 70A, Room 3377**

I will discuss the application of density functional based approaches to f state systems and in particular the use of the LDA+U extension to improve on the (LDA) local density approximation for f state systems. I will then present some applications of this approach to Eu- and Ce-doped gamma ray detector materials and lanthanide and actinide systems for energy critical materials.